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We have studied and developed procedures for the adaptive and parallel solution of transient partial differential equations. In particular, we concentrated on (i) techniques to manage distributed data, (ii) dynamic load balancing, (iii) discontinuous Galerkin schemes for hyperbolic systems, (iv) a posteriori error estimation strategies for discontinuous Galerkin methods, and (v) generalized mesh adaptation procedures. The resulting software is being applied to problems arising in several disciplines; however, it has been most successful with compressible fluid dynamics.

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Final Report

Adaptive and Parallel Computation for Transient Partial Differential Equations

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Abstract

We have studied and developed procedures for the adaptive and parallel solution of transient partial differential equations. In particular, we concentrated on (*i*) techniques to manage distributed data, (*ii*) dynamic load balancing, (*iii*) discontinuous Galerkin schemes for hyperbolic systems, (*iv*) *a posteriori* error estimation strategies for discontinuous Galerkin methods, and (*v*) generalized mesh adaptation procedures. The resulting software is being applied to problems arising in several disciplines; however, it has been most successful with compressible fluid dynamics.

1 Scientific Accomplishments

1.1 Introduction

We examined adaptive and parallel solution procedures for transient partial differential equations. In particular, we describe (*i*) libraries for managing distributed data, (*ii*) dynamic load balancing techniques, (*iii*) parallel algebraic solution procedures, (*iv*) discontinuous Galerkin methods for hyperbolic systems of conservation laws, (*v*) *a posteriori* error estimation for discontinuous Galerkin methods, and (*vi*) generalized mesh adaptation procedures.

1.2 Parallel Data Management

The *Rensselaer Partition Model* (RPM) [22, 21] is a hierarchical structure with a partition model containing the actual dissection of the domain into segments. Partitions are grouped by a process model for assignment to processes. Processes are assigned to a machine model that represents the actual computational nodes and their communication and memory properties. RPM's dynamic partitioning capabilities make it possible to tailor task scheduling to a particular architecture. Its structure is rich enough to handle h-, p-, and r-refinement and several discretization technologies, including finite difference, finite volume, finite element, and partition of unity methods.

RPM can manage distributed data and support multiple partitions per process and multiple mesh data structures. We are developing procedures that automatically gather and include data on computer processing, memory, and communications performance for use with load balancing on heterogeneous processing systems. These would greatly enhance the performance in such environments and improve the generality of the data management system.

1.3 Dynamic Load Balancing

Several modifications have been made to the distributed octree partitioning procedures to enhance their performance. These are described in the M.S. thesis of Paul Campbell [4] and include (*i*) capabilities to retain the octree between successive load balancings, (*ii*) improved performance of the various space filling curves used to traverse the octree structures, and (*iii*) a superior distribution algorithm. These facilities have been incorporated into Sandia National Laboratories' *Zoltan* dynamic load balancing library. The ability to save the distributed octree between load balancings avoids the need to re-build and distribute a tree at each load balancing and, additionally, improves scalability.

Different octree traversals offer superior performance in some instances. Our octree libraries have capabilities to traverse the distributed tree using Morton, Gray code, and Hilbert orderings [4]. Examples exist where each one provides the best performance [4]; however, in general, the Hilbert ordering is best. As an example, consider the adaptive solution of the flow in a vented shock tube [8] on a 56-processor IBM SP computer over a sequence of ten adaptive mesh refinements. Results in Figure 1 show the maximum and average surface communication indices and interprocessor adjacencies using Morton

and Hilbert tree traversals. The average surface index is the number of element faces on the boundaries of partitions relative to the total number of element faces in the problem. The maximum surface index provides similar information for each processor and then maximizes this data over the processors. These indices provide a measure of communications costs. The interprocessor adjacencies indicate the relative number of other processors to which a given processor must communicate. It provides a measure of message latency.

The results in Figure 1 indicate that the Hilbert ordering is superior to the Morton ordering for this problem. (The Gray code ordering was worse than these two in this case.) The initial mesh contained approximately 70,000 elements, the fifth mesh contained approximately 300,000 elements, and the tenth mesh contained in excess of 500,000 elements.

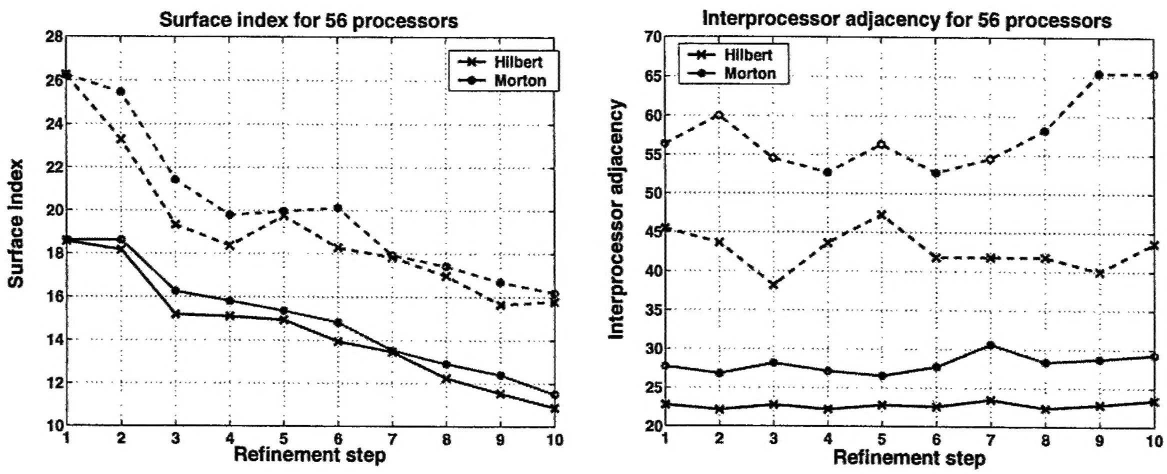

Figure 1: Surface indices and interprocessor adjacencies for ten rebalancings during a 56-processor adaptive finite element solution. Solid lines show average surface index (left) and interprocessor adjacency (right). The dashed lines show the maximum surface index (left) and interprocessor adjacency (right).

1.4 Solution Procedures

We have concluded our investigation of efficient, parallel, preconditioning methods for the solution of large, sparse, indefinite linear algebraic systems with the culmination of Turner's Ph.D. dissertation [23]. Two manuscripts based on this work have been submitted for publication [24, 25]. The techniques describe a multilevel (AMLI) preconditioning of Axelsson and Vassilevski applied to a quasi-minimum residual (QMR) iterative procedure. Coarsenings on unstructured meshes with adaptive h-refinement are provided by projecting the solutions onto an octree structure (*i.e.*, used for the load balancing) and then pruning the octree [25]. This is simpler than coarsening the original mesh and provides a readily available distributed structure.

Parallel procedures rely on the principles of generic programming to isolate the abstractions of matrices and vectors from their particular implementation as serial or parallel data objects. The goal is a standard such that any matrix or vector written to provide the required functionality can be used interchangeably [24]. The implementation relies heavily on operator overloading and function/object templates. The algebraic interface has been tested relative to several serial and parallel representations including compressed sparse row (CSR) storage and a block oriented recursive matrix format useful with AMLI preconditioning. Qualitatively, the results indicate that near transparent parallelism can be obtained if sufficient care is taken with the serial implementation.

1.5 Discontinuous Galerkin Procedures

The discontinuous Galerkin (DG) method offers several advantages relative to traditional finite element and finite volume methods when solving hyperbolic systems of conservation laws. It may be applied to arbitrarily high orders of accuracy on structured and unstructured meshes with a compact stencil. There is no need to enforce conformity and continuity in either the mesh or solution; thus, adaptive h- and p-refinement are greatly simplified. Inter element communication is face based, which simplifies parallel computation. Shock waves and other discontinuities are captured sharply to the nearest element boundary. And, conservation principles are satisfied on an element-by-element basis, which is important in many applications. These advantages and several aspects of the DG method are described in a sequence of manuscripts that construct orthogonal bases [16], describe limiting procedures [7], develop efficient local time stepping algorithms [18], create efficient serial and parallel data representations [17] and apply the method to compressible flow problems [7, 16, 17, 18].

In order to guide adaptive enrichment and appraise the accuracy of computed solutions, we developed *a posteriori* estimates of discretization errors. For one-dimensional systems, we have proven [3] that that the leading term of the spatial discretization error with piecewise-polynomial approximations of degree p is proportional to a Radau polynomial of degree $p+1$ on each element. With h a measure of the mesh spacing, we also prove that the spatial discretization error is $O(h^{2p+1})$ at the downwind point and $O(h^{p+2})$ at the remaining roots of Radau polynomial of degree $p+1$ on each element. These results are used to construct asymptotically correct *a posteriori* estimates of spatial discretization errors that are effective in regions where solutions are smooth. The strong "superconvergence" at the downwind element ends has enabled us to obtain these global rather than local error estimates.

Our results have been extended to multiple dimensions where we show that the leading term of the spatial discretization error of a piecewise-polynomial solution of degree p is the difference between orthogonal polynomials of degrees p and $p+1$ [14]. Since Radau polynomials are the difference between successive Legendre polynomials, our error estimate may be thought of as a multi-dimensional Radau polynomial. We further show that the strong superconvergence at downwind element boundaries persists in the sense that the average spatial error on downwind element faces converges as $O(h^{2p+1})$ [14].

N	16		56		160	
p	$\|e\|_0$	θ	$\|e\|_0$	θ	$\|e\|_0$	θ
0	4.85e-02	1.0116	2.49e-04	1.0304	1.49e-02	1.0418
1	8.27e-04	1.0022	2.16e-04	1.0537	7.85e-05	1.0266
2	3.11e-05	0.9609	4.16e-06	0.9267	9.24e-07	0.9054
3	1.71e-06	1.0161	1.04e-07	1.0546	1.47e-08	1.0054
4	1.07e-07	1.0597	3.32e-09	1.0097	2.8e-10	0.9203

Table 1: Errors $\|e\|_0$ and effectivity indices θ in the L_2 norm for the problem (1).

As an example, consider the solution of

$$2u_x + u_y = \frac{3}{2u} \tag{1a}$$

on the square $0 \leq x, y \leq 1$ with boundary conditions chosen so that the exact solution is

$$u = \sqrt{x + y + 1}. \tag{1b}$$

Computations were performed on unstructured meshes with $N = 16$, 56, and 160 elements and polynomial degrees $p = 0, 1, \ldots, 4$ [14]. Results for the discretization error in the L_2 norm and the effectivity index (ratio of the estimated to exact error in the L_2 norm) are presented in Table 1. All effectivity indices are within 10% of their ideal unit values.

We also report the rate of convergence on the outflow boundary by conducting a sequence of computations on meshes obtained by solving (1) on uniform right-triangular-element meshes that have diagonals running from the upper left to the lower right of the region [14]. Let

$$I^+ = \int_L (u - U^-)\, dt, \tag{2}$$

where L is the line connecting the upper left corner of the domain $(0, 1)$ to the lower right corner $(1, 0)$. Here, U^- is the numerical solution on the left of L; hence, we may interpret I^+ as the average error on outflow boundaries of those elements to the left of L. To compare, we also compute

$$I^- = \int_L (u - U^+)\, dt, \tag{3}$$

where U^+ is the numerical solution on the right of L. Thus, I^- may be interpreted as the average error on inflow boundaries of those elements to the right of L.

Results for $p = 0, 1, 2, 3$, and $N = 8, 32, 128$, are presented in Table 2. Estimates of the convergence rates compare well with the theoretical $O(h^{2p+1})$ and $O(h^{p+1})$ rates on outflow and inflow boundaries, respectively. The average numerical solution is, thus, considerably more accurate along an outflow edge than it is along an inflow edge, even for very coarse meshes.

We have observed that the strong superconvergence at outflow boundaries [14] can be used to identify discontinuities. This, in turn, can be used to provide information on where to apply limiting to reduce oscillations when using high-order methods.

	$p=0$				$p=1$			
N	I^-	r	I^+	r	I^-	r	I^+	r
8	1.08e-01	-	1.07e-02	-	2.23e-03	-	7.53e-06	-
32	5.57e-02	0.96	5.08e-03	1.07	6.02e-04	1.89	8.95e-07	3.07
128	2.11e-02	1.4	2.47e-03	1.04	1.56e-04	1.95	1.09e-07	3.04
	$p=2$				$p=3$			
N	I^-	r	I^+	r	I^-	r	I^+	r
8	7.56e-05	-	1.98e-08	-	3.02e-06	-	8.26e-11	-
32	1.07e-05	2.82	4.83e-10	5.35	2.25e-07	3.74	6.17e-13	7.06
128	1.43e-06	2.93	1.77e-11	4.77	1.55e-08	3.85	5.44e-15	6.82

Table 2: Average errors on inflow I^- and outflow I^+ boundaries L for (1) as functions of p and N and estimated convergence rates r.

1.6 Generalized Mesh Adaptation Procedures

Procedures to adaptively refine meshes are well known in the case of straight sided, planar-faced elements. However, the application of these techniques to three-dimensional domains will not improve the geometric approximation when the domain is curved. The simple "snapping" of nodes to the curved boundary can yield invalid elements. Therefore, a procedure is needed to perform mesh adaptation for curved three-dimensional domains that explicitly considers the snapping of vertices to curved domain boundaries. The procedure begins by applying a set of refinement templates appropriate for straight sided, planar-faced elements. At this point the mesh topology is what was requested by the adaptive procedure. However, the geometry of the mesh is incorrect for the new mesh vertices classified on curved domain boundaries.

The procedure to place refinement vertices on the model boundary employs mesh modification operators when moving the vertex to the boundary would yield invalid or unacceptably shaped elements. The first step in the algorithm when a vertex can not be moved is to determine the first plane which, if crossed, causes one or more elements to become invalid. With this information, consideration is given to the mesh modification(s) needed to ensure the vertex can be moved onto that plane or past. If after that modification the mesh vertex can be placed at an appropriate boundary point, it is and that vertex needs no further consideration. If that vertex is still not on the boundary, it is placed back into the list to be considered again after the others are attempted. If this process is not successful in placing all the vertices on the boundary, a local cavity is created with its vertices on the boundary as appropriate and the cavity is given to a cavity meshing procedure. Since the cavity mesher can create new boundary vertices that are placed on a local faceted approximation of the boundary, it is possible to create new vertices that also have to be moved to the boundary. Typically the number of these new points is low (or zero) and they are usually closer to the boundary than the previously considered points. Further details appear in Li *et al.* [15]

In the adaptive simulation of evolving geometry problems local mesh enrichments are requested to refined/coarsened elements to account for discretization error control, and/or

improve their shapes which have degraded due to large deformations. A combined mesh enrichment process is being developed to most effectively address both considerations. The mesh enrichments are executed through the controlled application of mesh entity swap, split, collapse and reposition operations [20]. Mesh refinement is accomplished using splitting operations with edge splits having the most flexibility. Mesh entity shape improvement is accomplished by node-point motion or the application swap, split and collapse operations. In simulations where the mesh to be modified after a specific analysis step contains general combinations of elements to be refined/coarsened and to have their shapes improved, it is possible to determine local mesh modifications that simultaneously consider the desired size and shape. The key new capability developed is the consideration of the best combination of local mesh modifications to execute when elements are to be both refined/coarsened and have their shape improved. The determination of which elements need shape improvement is based on one of the standard non-dimensional isotropic shape measures. However, the algorithms to select the appropriate shape modifications consider more detailed information on the element shape (dihedral angles and edge lengths) and element refinement/coarsening information in the selection process.

2 Scientific Personnel

In addition to the Principal Investigators Joseph E. Flaherty and Mark S. Shephard, former Ph.D. scholars James Teresco and Wesley Turner and M.S. student Paul Campbell were supported by this project. Current Ph.D. students Lilia Krivodonova and Peng Hu have also received support. Krivodonova is expected to complete her Ph.D. dissertation this spring.

3 Technology Transfer

3.1 Interactions

Joseph E. Flaherty and Mark S. Shephard have regular interactions with Robert Dillon, Deborah Bleau, and Daniel Cler of Benét Laboratories. We have been collaborating on using the DG software to analyze muzzle blast effects with large-calibre weapons systems. These problems involve complex three-dimensional interior and exterior flows including realistic geometries and ground reflections.

A start-up company, Simmetrix Corporation, is building on the mesh modification and analysis framework developments done in this project. Simmetrix has built upon the analysis framework developments to obtain Phase II DOE and AFOSR SBIR grants, of which Rensselaer has subcontracts for some of the further development.

The octree load balancing software has been incorporated into the Zoltan dynamic load balancing library of Sandia National Laboratory.

3.2 Presentations

1. J.E. Flaherty, "Parallel adaptive computation using discontinuous Galerkin methods, Department of Applied Mathematics, Brown University, Providence, February 11, 2000.

2. M.S. Shephard, "Automation of large-scale simulations with emphasis on geometry-based issues," Technische Universitat Munchen, Fakultat f ur Bauingenieur und Vermessungswesen, Munich, March 6, 2000.

3. M.S. Shephard, "Automation of large-scale simulations with emphasis on geometry-based issues," Universitat Stuttgart, Institut f ur Baustatik, Stuttgart, March 7, 2000.

4. M.S. Shephard, "Mesh adaption for curved domains," Workshop on Adaptive FEM in Computational Mechanics, Institute for Structural and Numerical Mechanics, Universitat Hannover, Hannover, March 9, 2000.

5. J.E. Flaherty, "Parallel adaptive solution of conservation laws by a discontinuous Galerkin method," workshop on *A Posteriori Error Estimation and Adaptive Approaches in the Finite Element Method*, Mathematical Sciences Research Institute, University of California Berkeley, Berkeley, April 3 - 14, 2000.

6. M.S. Shephard, "Automation of large-scale simulations with emphasis on geometry-based issues," Department of Mechanical Engineering, Carnegie Mellon University, Pittsburgh, April 28, 2000.

7. J.E. Flaherty, "Software for parallel adaptive DG computation," special session on Discontinuous Galerkin Methods, Conference on *Finite Elements in Flow Problems 2000*, The University of Texas at Austin, Austin, April 30 - May 4, 2000.

8. J.E. Flaherty, "Architecture-dependent finite element computation using the Rensselaer Partition Model" and "Adaptive discontinuous Galerkin method with an orthonormal basis," Mini-Symposium on Parallel Adaptive Computations, Conference on *p and hp Finite Element Methods: Mathematics and Engineering Practice (p-FEM 2000)*, Washington University, St. Louis, May 31 - June 2, 2000.

9. M.S. Shephard, "Trellis - A geometry based adaptive analysis framework for a multi-processor environment" and "Algorithm to generate p-version meshes for curved domains," *p and hp Finite Element Methods: Mathematics and Engineering Practice (p-FEM 2000)*, Washington University, St. Louis, May 31 - June 2, 2000.

10. J.E. Flaherty, "Software for Parallel Adaptive Computation" and "A Posteriori Error Estimation for the Discontinuous Galerkin Method," Sandia National Laboratory, Albuquerque, June 21, 22, 2000.

11. J.E. Flaherty, "Software for Parallel Adaptive Computation," organized session on Adaptive Techniques for PDEs, *16th IMACS World Congress 2000*, Lausanne, August 20 - 25, 2000.

12. J.E. Flaherty, "Adaptive Discontinuous Galerkin Methods for Conservation Laws," Department of Computer Science, William and Mary College, Williamsburg, September 13, 2000.

13. M.S. Shephard, "Mesh adaption for curved domains," SIAM Conference on Scientific Computing, Washington, September 24, 2000.

14. J.E. Flaherty, "Parallel adaptive computation using discontinuous Galerkin methods," Mathematical and Computational Sciences Division, National Institute of Standards and Testing, Gaithersburg, September 26, 2000.

15. M.S. Shephard, "Automated modeling technologies," MASC Advisory Board Meeting, United Technologies Research Center, Hartford, January 15, 2001.

16. M.S. Shephard, "Automatic mesh generation for geometry-based simulation", keynote lecture at the *17th GAMM Seminar on Construction of Grid Generation Algorithms*, Max-Planck-Institute for Mathematics in the Sciences, Leipzig, February 1, 2001.

17. J.E. Flaherty, "Parallel adaptive computation using discontinuous Galerkin methods," Department of Mathematical Sciences, University of Nevada at Las Vegas, Las Vegas, February 8, 2001.

18. M.S. Shephard, "Simulation-based design," The Boeing Company, Long Beach, March 27, 2001.

19. J.E. Flaherty, "Discontinuous Galerkin methods for hyperbolic conservation laws," Robert J. Melosh Lecture, Department of Civil and Environmental Engineering, Duke University, Durham, March 30, 2001.

20. J.E. Flaherty, "Discontinuous Galerkin methods for conservation laws," workshop on *Numerical Methods for Singular Perturbation Problems*, Mathematisches Forschungsinstitut Oberwolfach, Oberwolfach, April 8-14, 2001.

21. M.S. Shephard, "Automation of large-scale simulations with emphasis on a flexible discontinuous Galerkin procedure," Annual Computational Science and Engineering Research Symposium, Center for the Simulation of Advanced Rockets, University of Illinois, Urbana-Champaign, April 20, 2001.

22. J.E. Flaherty, "A hierarchical data management system for parallel partitioning of adaptive computation," *The Conference on High Speed Computing*, Salishan Lodge, Gleneden Beach, April 23-26, 2001.

23. J.E. Flaherty, "A hierarchical data management system for parallel partitioning of adaptive computation," Sun Microsystems, Burlington, May 3, 2001.

24. J.E. Flaherty, "Adaptive and Parallel Discontinuous Galerkin Methods for Hyperbolic Systems," International Conference on Computational Mathematics, Pohang, South Korea, July 2 - July 5, 2001.

25. L. Krivodonova, "A Posteriori Error Estimation for Discontinuous Galerkin Method," invited poster presentation, American Women in Mathematics Workshop, *SIAM National Meeting*, San Diego, July 9 - 13, 2001.

26. J.E. Flaherty, "Discontinuous Galerkin Methods for Conservation Laws," Minisymposium on Adaptive Grids in Differential Equations, *International Conference on Scientific Computation and Differential Equations*, Vancouver, July 29 - August 3, 2001.

27. L. Krivodonova, "Error Estimation for Discontinuous Galerkin Method," Minisymposium on Discontinuous Galerkin Methods", *Sixth U.S. National Congress on Computational Mechanics*, Dearborn, August 1 - 3, 2001.

28. J.-F. Remacle, "Three Dimensional Parallel Adaptive Discontinuous Galerkin Method for Solving Conservation Laws," Minisymposium on Discontinuous Galerkin Methods, *Sixth U.S. National Congress on Computational Mechanics*, Dearborn, August 1 - 3, 2001.

29. L. Krivodonova, "Limiting Techniques and Error Estimation for Hyperbolic Conservation Laws," poster presentation at *Frontiers in Information Technology Symposium on Multiscale Computation*, Rensselaer Polytechnic Institute, Troy, November 8, 2001.

30. J.E. Flaherty, "Adaptive and Parallel Discontinuous Galerkin Methods for Hyperbolic Systems," Research Institute in Advanced Computer Science (RIACS), NASA Ames Research Center, Moffett Field, January 9, 2002.

31. J.E. Flaherty, "Adaptive and Parallel Discontinuous Galerkin Methods for Hyperbolic Systems," Institute of Mathematical Sciences, Chinese University of Hong Kong, Hong Kong, March 6, 2002.

4 List of Manuscripts

A list of manuscripts that were submitted, accepted, or appeared under this contract follows.

[1] S. Adjerid, M. Aiffa, and J. E. Flaherty. Hierarchical finite element bases for triangular and tetrahedral elements. *Computer Methods in Applied Mechanics and Engineering*, 190:2925–2941, 2001.

[2] S. Adjerid, B. Belguendouz, and J. E. Flaherty. A posteriori finite element error estimation for diffusion problems. *SIAM Journal on Scientific Computing*, 2001. to appear.

[3] S. Adjerid, K.D. Devine, J.E. Flaherty, and L. Krivodonova. A posteriori error estimation for discontinuous Galerkin solutions of hyperbolic problems. *Computer Methods in Applied Mechanics and Engineering*, 191:1997–1112, 2002.

[4] Paul M. Campbell. The performance of an octree load balancer for parallel adaptive finite element computation. Master's thesis, Computer Science Department, Rensselaer Polytechnic Institute, Troy, 2001.

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[14] L. Krivodonova and J.E. Flaherty. Error estimation for discontinuous Galerkin solutions of multidimensional hyperbolic problems. *Advances in Computational Mathematics*, submitted, 2001.

[15] X. Li, M.S. Shephard, and M.W. Beall. Accounting for curved domains in mesh adaptation. *International Journal for Numerical Methods in Engineering*, to appear, 2002.

[16] J.-F. Remacle, J. E. Flaherty, and M. S. Shephard. An adaptive discontinuous Galerkin technique with an orthogonal basis applied to Rayleigh-Taylor flow instabilities. *SIAM Review*, submitted, 2000.

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